

Butanoic acid, 2-hydroxy-3-methyl-, ethyl ester

Other names:	Butyric acid, 2-hydroxy-3-methyl-, ethyl ester Ethyl 2-hydroxyisovalerate Ethyl 2-hydroxy-3-methylbutanoate Ethyl 2-hydroxy-3-methylbutyrate
Inchi:	InChI=1S/C7H14O3/c1-4-10-7(9)6(8)5(2)3/h5-6,8H,4H2,1-3H3
InchiKey:	IZRVEUZYBVGFC-UHFFFAOYSA-N
Formula:	C7H14O3
SMILES:	CCOC(=O)C(O)C(C)C
Mol. weight [g/mol]:	146.18
CAS:	2441-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-367.56	kJ/mol	Joback Method
hf	-595.40	kJ/mol	Joback Method
hfus	13.71	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.566		Crippen Method
mcvol	122.800	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	987.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	987.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1445.00		NIST Webbook
ripol	1422.00		NIST Webbook
ripol	1403.00		NIST Webbook

ripol	1399.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1399.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1426.00		NIST Webbook
ripol	1411.00		NIST Webbook
ripol	1430.00		NIST Webbook
ripol	1421.00		NIST Webbook
ripol	1427.30		NIST Webbook
ripol	1422.00		NIST Webbook
tb	527.15	K	Joback Method
tc	703.42	K	Joback Method
tf	271.63	K	Joback Method
vc	0.459	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.08	J/molxK	527.15	Joback Method
cpg	336.78	J/molxK	674.04	Joback Method
cpg	328.05	J/molxK	644.66	Joback Method
cpg	318.91	J/molxK	615.28	Joback Method
cpg	309.37	J/molxK	585.91	Joback Method
cpg	299.43	J/molxK	556.53	Joback Method
cpg	345.13	J/molxK	703.42	Joback Method
dvisc	0.0001175	Paxs	527.15	Joback Method
dvisc	0.0001982	Paxs	484.56	Joback Method
dvisc	0.0003695	Paxs	441.98	Joback Method
dvisc	0.0007868	Paxs	399.39	Joback Method
dvisc	0.0020069	Paxs	356.80	Joback Method
dvisc	0.0065975	Paxs	314.22	Joback Method
dvisc	0.0314993	Paxs	271.63	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2441067&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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